

# The nonlinear heat equation on dense graphs and graph limits

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## Abstract

The continuum (thermodynamic) limit is the most important tool for analyzing pattern formation in large networks of dynamical systems with nonlocal coupling. In this limit, the solutions of the initial value problems for evolution equations on large discrete networks are approximated by those for the limiting integro-differential equations posed on continuous spatial domains. While this limiting procedure plays a pivotal role in elucidating the mechanisms of some very important effects such as chimera states, multistability, synchronization, and the coherence-incoherence transition, its mathematical basis remains little understood. In this paper, we use the combination of the ideas and results of the theory of graph limits and techniques for nonlinear evolution equations to provide a rigorous mathematical justification for taking the continuum limit and to extend this method to cover many complex networks, for which it has not been applied before. Specifically, for dynamical networks on convergent sequences of simple and weighted graphs, we prove convergence of solutions of the IVPs for discrete models to those of the limiting continuous equations. In addition, for sequences of simple graphs that converge to  $\{0, 1\}$ -valued graphons, we show that the rate of convergence depends on the fractal dimension of the boundary of the support of the graph limit. The results of this paper are used to study the regions of continuity of chimera states and the attractors of the nonlocal Kuramoto equation on certain bipartite graphs.

## 1 Introduction

Systems of nonlocally coupled oscillators have been a subject of intense research during the last decade due to the intricate new dynamics found in these models and their importance in applications. Nonlocally coupled systems arise in modeling diverse physical, biological, and technological systems. Examples include neuronal models [16, 2, 33], models of pattern-forming systems [26, 34], models of the spread of disease [22], those of coupled lasers [17], and Josephson junctions [30, 35], and power networks [9], to name a few. Compared to systems with local (diffusive) coupling [8], dynamical mechanisms for pattern formation in nonlocal systems are much less understood.

The continuum (thermodynamic) limit proved to be a very important and versatile tool for analyzing pattern formation in large networks of dynamical systems with nonlocal coupling [15, 1, 37, 29, 13, 28, 27].

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In this limit, the solutions of the initial value problems (IVPs) for evolution equations on large discrete networks are approximated by those for the limiting integro-differential equations posed on continuous spatial domains. This limiting procedure plays a pivotal role in elucidating the mechanisms of some very important effects such as chimera states [15, 1], multistability [37, 13], synchronization, and the coherence-incoherence transition [28].

To set the stage for the forthcoming analysis of the thermodynamic limit in the nonlocally coupled systems, we first review a representative application. In [37], Wiley, Strogatz, and Girvan studied a nonlocally coupled system of phase oscillators

$$\dot{\phi}_i = \omega + \frac{1}{n} \sum_{j=i-k}^{i+k} \sin(\phi_j - \phi_i), \quad (1.1)$$

where  $\phi_i : \mathbb{R}^+ \rightarrow \mathbb{S}^1 := \mathbb{R}/2\pi\mathbb{Z}$ ,  $i \in [n] := \{1, 2, 3, \dots, n\}$  is interpreted as the phase of oscillator  $i$ ,  $\omega$  is the intrinsic frequency, and the sum models the interactions between oscillator  $i$  and  $k$  of its nearest neighbors from each side (cf. [14, 15]). It is assumed that the oscillators are located on a ring and indexed by integers  $\mathbb{Z}/n\mathbb{Z}$ .

It is instructive to view (1.1) as a system of differential equations on graph  $G_n = \langle V(G_n), E(G_n) \rangle$  with the vertex set  $V(G_n) = [n]$  and the edge set

$$E(G_n) = \{(i, j) \in [n]^2 : \text{dist}(i, j) \leq k\} \text{ where, } \text{dist}(i, j) = \min\{|i - j|, n - |i - j|\}.$$

Let  $W_{G_n} : [0, 1]^2 \rightarrow \{0, 1\}$  such that

$$W_{G_n}(x, y) = 1 \text{ if } (i, j) \in E(G_n) \text{ and } (x, y) \in [(i-1)n^{-1}, in^{-1}) \times [(j-1)n^{-1}, jn^{-1}).$$

The plot of function  $W_{G_n}(x, y)$  in Fig. 1a provides the pixel picture of the adjacency matrix of  $G_n$ . In Fig. 1a and in similar plots throughout this paper, we place the origin of the unit square in the top left corner of the plot to emphasize the correspondence between  $W_{G_n}$  and the adjacency matrix of  $G_n$ . As  $n \rightarrow \infty$ ,  $\{W_{G_n}\}$  converges to  $W_G(x, y)$  (see Fig. 1b).

In [37], the analysis of the attracting states of (1.1) employs the continuum limit of (1.1). To this end, let  $k = rn$  for some fixed  $r \in (0, 1]$ , and send  $n \rightarrow \infty$ . Then in the uniformly rotating frame of coordinates (1.1) formally becomes

$$\frac{\partial}{\partial t} \phi(x, t) = \int_I W_G(x, y) \sin(\phi(y, t) - \phi(x, t)) dy \text{ as } n \rightarrow \infty, \quad (1.2)$$

where  $\phi(x, t)$  describes the evolution of the continuum of oscillators distributed over  $I$ . Throughout this paper,  $I$  denotes  $[0, 1]$ , the spatial domain of the continuous limits of the dynamical networks. Equation (1.2) is called the thermodynamic limit of (1.1). From (1.2), it is easy to find a family of steady state solutions

$$\theta^{(q)}(x, t) = qx + c, \quad q \in \mathbb{Z}, \quad c \in \mathbb{R},$$

so-called  $q$ -twisted states, and study effectively their linear stability (cf. [37]). This information is then used to infer about the attracting states of the discrete system (1.1) for large  $n \gg 1$ .

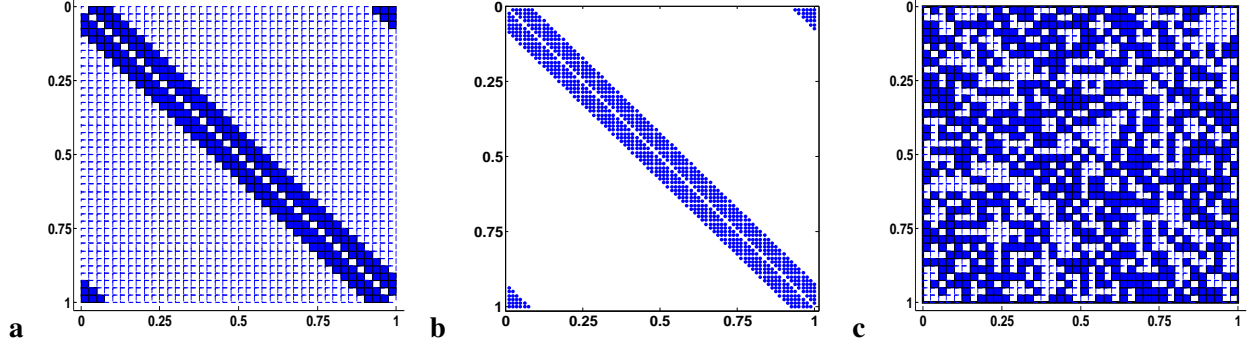


Figure 1: The plot of  $W_{G_n}$  (a) and its limit  $W_G$  (b). c The plot of  $W_{G(n,p)}$ . Each function is defined on a unit square and is equal to 1 on regions colored in black and 0 otherwise.

Following the same lines Girnyk, Maistrenko, and Hasler studied the Kuramoto model with repelling coupling [13]

$$\dot{\theta}_i = \omega - n^{-1} \sum_{j=i-k}^{i+k} \sin(\theta_j - \theta_i). \quad (1.3)$$

Interestingly, along with the  $q$ -twisted states in this model they found attracting states with more complex spatial organization, multi-twisted states, that were not present in the original model (1.1).

In the analysis of either model the use of the continuum limit was instrumental. However, these examples raise the following questions.

- (A) Does the continuum model (1.2) truly approximate the dynamics of the discrete model (1.1) for large finite  $n$ ? If so, in what sense the solutions of the integro-differential equation approximate those of (1.1)?
- (B) How big is the class of network topologies for which one can use the continuum limit? Is it restricted to special graphs like  $k$ -nearest neighbor coupling on a ring? Can it be applied for instance to the small world networks, the original motivation for the analysis in [37]?

The function  $W_G$  shown in Fig. 1b is the limit of the functions  $W_{G_n}$  (Fig. 1a) representing the adjacency matrices of the  $k$ -nearest neighbor family of graphs  $\{G_n\}$ . The latter is an example of a convergent graph sequence and  $W_G$  is the corresponding graph limit [18]. This observation hints on the relevance of the theory of graph limits for constructing the continuum limits for dynamical networks. In the remainder of this paper, we use the combination of the ideas and results of the theory of graph limits [5, 4, 19, 20, 21], and techniques for nonlinear evolution equations [6, 10] to provide a rigorous mathematical justification for taking the continuum limit and to extend this method to cover many complex networks, for which it has not been applied before.

This paper is organized as follows. We review the necessary background on graph limits in Section 2. In Section 3, we discuss the heat equation on graphs and graph limits. Here, we extend a classical linear heat equation on graphs to allow nonlinear diffusion. This extension covers many dynamical networks arising in applications including coupled oscillator models like (1.1). In the same section, we formally define the

continuum limit for dynamical networks of a convergent sequence of dense (weighted) graphs. In this limit, the discrete diffusion operator becomes an integral operator with the kernel representing the limit of the infinite family of graphs. We show that the IVP for the limiting equation is well-posed and admits a unique solution in  $C(0, T; L^\infty(I))$ . Further, in Theorem 3.2, we specify conditions on the kernel and the initial conditions, which guarantee that the solutions of the IVPs remain continuous in space over subdomains of  $I$ . This result is used to characterize the attractors of the continuum model. In particular, we apply it to study the regions of continuity of the chimera states and attractors of the Kuramoto equation on the half graph (see Section 6). The rest of the paper is focused on studying the relation between the solutions of the IVPs for discrete networks and those for the corresponding limiting integro-differential equations. To this end, In Section 4, for sequences of simple graphs converging to  $\{0, 1\}$ -valued graphons, we show that the rate of convergence depends on the fractal dimension of the boundary of support of the graph limit. This shows explicitly how the geometry of the graphon affects the accuracy of the continuum limit. In Section 5, we analyze networks on convergent weighted graph sequences. The results of this paper are illustrated with the discussion of the dynamics of two concrete models: the Kuramoto-Battogtokh nonlocal system generating chimera states [15] and the Kuramoto equation on the half and complete bipartite graphs (cf. Section 6). The final section, Section 7, contains concluding remarks and the outlook on future work.

## 2 Graph limits

In this section, we review several definitions and results from the theory of graph limits that we will need later. In our brief tour through graph limits, we mainly follow [3] and [31]. For the full exposition of this powerful theory with many diverse applications, we refer an interested reader to the pioneering papers by Lovász and Szegedy [19, 20], and Borgs, Chayes, Lovász, Sós, and Vesztegombi [5, 4]; and to the monograph [18].

Undirected graph  $G = \langle V(G), E(G) \rangle$  without loops and multiple edges is called simple.  $V(G)$  stands for the set of nodes and  $E(G) \subset V(G) \times V(G)$  denotes the edge set.

The convergence of a sequence of simple graphs  $G_n = \langle V(G_n), E(G_n) \rangle$  is defined in terms of the homomorphism densities

$$t(F, G_n) = \frac{\text{hom}(F, G_n)}{|V(G_n)|^{|V(F)|}}, \quad (2.1)$$

where  $\text{hom}(F, G_n)$  is the number of homomorphisms (i.e., adjacency preserving maps  $V(F) \rightarrow V(G_n)$ ). The probabilistic interpretation of (2.1) is the probability of a random map  $h : V(F) \rightarrow V(G_n)$  to be a homomorphism.

**Definition 2.1.** [19, 4] *The sequence of graphs  $\{G_n\}$  is called convergent if  $t(F, G_n)$  is convergent for every simple graph  $F$ .<sup>1</sup>*

It turns out that the limiting object can be represented by a measurable symmetric function  $W : I^2 \rightarrow I$ . We recall that  $I$  stands for  $[0, 1]$ . Such functions are called graphons and the set of all graphons is denoted by  $\mathcal{W}_0$ .

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<sup>1</sup>In the theory of graph limits, convergence in Definition 2.1 is called left-convergence. Since this is the only convergence of graph sequences used in this paper, we refer to the left-convergent sequences as convergent.

**Theorem 2.2.** [19] *For every convergent sequence of simple graphs there is a graphon  $W \in \mathcal{W}_0$  such that*

$$t(F, G_n) \rightarrow t(F, W) := \int_{I^{|V(F)|}} \prod_{ij \in E(F)} W(x_i, x_j) dx \quad \forall F. \quad (2.2)$$

*Moreover, for every  $W \in \mathcal{W}_0$  there is a convergent sequence of graphs satisfying (2.2).*

In the analytical description of graph limits, the notion of cut-norm of a graphon plays a central role. While this norm is not used explicitly in the analysis of the dynamical networks below, it is crucial for understanding of the metric properties of graphons. For any integrable function  $W$ , the cut-norm is defined by

$$\|W\|_{\square} = \sup_{S, T \in \mathcal{L}_I} \left| \int_{S \times T} W(x, y) dx dy \right|,$$

where  $\mathcal{L}_I$  stands for the set of all Lebesgue measurable subsets of  $I$ . The cut-distance between two graphons  $W$  and  $U$  is defined by

$$\delta_{\square}(U, W) = \inf_{\phi \in \Phi} \|U - W^{\phi}\|_{\square}.$$

respectively. Here,  $\Phi$  denotes the set of measure-preserving bijections  $\phi : I \rightarrow I$  and  $W^{\phi}(x, y) := W(\phi(x), \phi(y))$  (see [4, 18] for a combinatorial definition of the cut-distance between graphs). A graph sequence is convergent if and only if it is Cauchy in the cut-distance [4].

Graph limits are the equivalence classes of graphons

$$[W] = \{U \in \mathcal{W}_0 : \delta_{\square}(U, W) = 0\}.$$

With a customary abuse of notation, we refer to both  $W$  and  $[W]$  as graphons. The pseudo-metric  $\delta_{\square}(\cdot, \cdot)$  induces the metric on  $\chi = \{[W] : W \in \mathcal{W}_0\}$ . The metric space  $(\chi, \delta_{\square})$  is compact [20].

In spite of a rather technical definition of a graphon, it admits a simple visual interpretation. Let  $G$  be a simple graph on  $n$  nodes,  $V(G) = [n]$ . Define

$$W_G(x, y) = \begin{cases} 1, & \text{if } (i, j) \in E(G) \text{ and } (x, y) \in \left[\frac{i-1}{n}, \frac{i}{n}\right) \times \left[\frac{j-1}{n}, \frac{j}{n}\right), \\ 0, & \text{otherwise.} \end{cases} \quad (2.3)$$

Then  $[W_G]$  is the graphon corresponding to  $G$ . Note that  $[W_G]$  is invariant under relabeling the nodes of  $G$  while  $W_G$  is not.  $W_G$  provides the pixel picture of the adjacency matrix of  $G$ . This is how we represented the adjacency matrix of the  $k$ -nearest-neighbor network in Fig. 1a (see [18] for more examples).

**Example 2.3.** [19, 4] *The Erdős-Renyi graphs. Consider a sequence of random graphs  $G(n, p) = \langle V(G(n, p)), E(G(n, p)) \rangle$ ,  $V(G(n, p)) = [n]$  such that  $\mathbb{P}\{(i, j) \in E(G(n, p))\} = p$  for any  $(i, j) \in [n]^2$ . This is a convergent sequence. The limit is the graphon  $[W]$  corresponding to the constant function  $W(x, y) = p$  for all  $(x, y) \in I^2$ . The pixel picture of  $W_{G(n, p)}$  is shown in Fig. 1c. The constant graphon  $W$  captures the limiting density of connections in  $G(n, p)$  for large  $n$ . Using the law of large numbers, it is easy to show that  $\|W_{G(n, p)} - p\|_{\square} \rightarrow 0$  as  $n \rightarrow \infty$ . Note that  $\{W_{G(n, p)}\}$  is not convergent in  $L^1$ -norm. This highlights the importance of the cut-norm in the analysis of graph limits.*

**Example 2.4.** [19] *The  $W$ -random graphs.* Let  $W \in \mathcal{W}_0$  and consider  $G_n = \langle [n], E(G_n) \rangle$  such that

$$\mathbb{P} \{ (i, j) \in E(G_n) \} = W \left( \frac{i}{n}, \frac{j}{n} \right).$$

*This is a convergent sequence. The limit is  $[W]$ . This simple construction provides a rich family of random graphs, whose limits are known explicitly. This example shows that for any measurable function  $W \in \mathcal{W}_0$ , there is a sequence of simple graphs  $G_n$  converging to  $[W]$ .*

**Example 2.5.** [19] *The half-graphs.* Let  $H_{n,n} = \langle V(H_{n,n}), E(H_{n,n}) \rangle$  be a bipartite graph on  $2n$  nodes such that

$$V(H_{n,n}) = \{1, 2, \dots, n, 1', 2', \dots, n'\}, \quad E(H_{n,n}) = \{(i, j') \in V(H_{n,n}) \times V(H_{n,n}) : i \leq j\}.$$

*The sequence  $\{H_{n,n}\}$  converges to the graphon  $[H]$  where  $H : I^2 \rightarrow I$  is the characteristic function of the set  $\{(x, y) : |x - y| \geq 1/2\}$ .*

### 3 The formulation of the problem

#### 3.1 The heat equation on discrete and continuous domains

Let  $G_n = \langle V(G_n), E(G_n), W(G_n) \rangle$  be a sequence of weighted graphs, where  $V(G_n) = [n]$  and  $E(G_n)$  are the set of nodes and edges respectively. Symmetric matrix  $W(G_n) : [n]^2 \rightarrow [-1, 1]$  to every edge  $(i, j) \in E(G_n)$  assigns a weight

$$(W(G_n))_{i,j} = \begin{cases} w_{ij}^{(n)} \in [-1, 1], & \text{if } (i, j) \in E(G_n), \\ 0, & \text{otherwise.} \end{cases}$$

If  $G_n$  is a simple graph,  $W(G_n)$  is a  $\{0, 1\}$ -valued matrix.

By the nonlinear heat equation on  $G_n$  we mean

$$\frac{d}{dt} u^{(n)}(t) = \lambda_i^{(n)} \sum_{j=1}^n w_{ij}^{(n)} D \left( u_j^{(n)} - u_i^{(n)} \right), \quad (3.1)$$

where  $u^{(n)}(t) = \left( u_1^{(n)}(t), u_2^{(n)}(t), \dots, u_n^{(n)}(t) \right)^\top$ ,  $\lambda_i^{(n)}$  are scaling coefficients. Function  $D : \mathbb{R} \rightarrow \mathbb{R}$  is Lipschitz continuous

$$|D(u) - D(v)| \leq L |u - v| \quad \forall u, v \in \mathbb{R}^1. \quad (3.2)$$

Throughout this paper, we will use  $\lambda_i^{(n)} = n^{-1}$ . However, other scalings may also be used.

If  $D(u) = u$  the coupling operator on the right-hand side of (3.1) is the graph Laplacian, and Equation (3.1) becomes the linear heat equation on  $G_n$ . The linear heat equation has many applications in combinatorial problems such as random walks on graphs [7], and dynamical problems, e.g., analysis of consensus protocols [23]. In this paper, we focus on the nonlinear heat equation, which provides the framework for a

large class of dynamical networks. In particular, the discrete Kuramoto equation (1.3), which we discussed in the Introduction, is of this type.

In the remainder of this paper, for a class of discrete problems (3.1), we will derive and justify the continuum counterpart of (3.1)

$$\frac{\partial}{\partial t} u(x, t) = \int_I W(x, y) D(u(y, t) - u(x, t)) dy. \quad (3.3)$$

The kernel  $W$  will be specified separately for each class of problems that we consider below.

### 3.2 The well-posedness of the IVP

Before we set out to study the relation between solutions of the discrete and continuous heat equations (3.1) and (3.3), we first address the well-posedness of the IVP for (3.3).

It is convenient to interpret the solution of the IVP for (3.3),  $u(x, t)$ , as a vector-valued map  $\mathbf{u} : [0, T] \rightarrow L^\infty(I)$ . Throughout this paper, we will use the bold font to denote the vector-valued function  $\mathbf{u}(t)$  corresponding to a function of two variables  $u(x, t)$ .

**Theorem 3.1.** *Suppose  $D(\cdot)$  is Lipschitz continuous,  $W \in L^\infty(I^2)$ , and  $\mathbf{g} \in L^\infty(I)$ . Then for any  $T > 0$ , there exists a unique solution of the IVP for (3.3)  $\mathbf{u} \in C^1(\mathbb{R}; L^\infty(I))$  subject to the initial condition  $\mathbf{u}(0) = \mathbf{g}$ .*

*Proof.* We rewrite the IVP for (3.3) as the integral equation

$$\mathbf{u}(t) = \mathbf{g} + \int_0^t \int_I W(x, y) D(u(y, t) - u(x, t)) dy dt =: [K\mathbf{u}](x, t). \quad (3.4)$$

Let  $M_{\mathbf{g}}$  be a metric subspace of  $C(0, \tau; L^\infty(I))$  (where  $\tau > 0$  will be specified later) consisting of functions  $\mathbf{u}$  satisfying  $\mathbf{u}(0) = \mathbf{g}$ . Then (3.4) is the fixed point equation for the operator  $K : M_{\mathbf{g}} \rightarrow M_{\mathbf{g}}$ . Without loss of generality, let  $\|W\|_{L^\infty(I^2)} = 1$ . We show below that  $K$  is a contraction for a small  $\tau > 0$ .

Indeed, let

$$\tau \leq (4L)^{-1}, \quad (3.5)$$

where  $L$  is the Lipschitz constant of  $D(\cdot)$ . For any  $\mathbf{u}, \mathbf{v} \in M_{\mathbf{g}}$  we have

$$\begin{aligned} \|K\mathbf{u} - K\mathbf{v}\|_{M_{\mathbf{g}}} &= \max_{t \in [0, \tau]} \|K\mathbf{u}(t) - K\mathbf{v}(t)\|_{L^\infty(I)} \\ &\leq \max_{t \in [0, \tau]} \operatorname{ess\,sup}_{x \in I} \left| \int_{I \times [0, t]} |W(x, y)| |D(u(y, t) - u(x, t)) - D(v(y, t) - v(x, t))| dy dt \right| \\ &\leq \tau L \max_{t \in [0, \tau]} \left\{ \int_I |u(y, t) - v(y, t)| dy + \|\mathbf{u}(t) - \mathbf{v}(t)\|_{L^\infty(I)} \right\} \\ &\leq 2\tau L \max_{t \in [0, \tau]} \|\mathbf{u}(t) - \mathbf{v}(t)\|_{L^\infty(I)}. \end{aligned}$$

Thus, by (3.5) we have

$$\|K\mathbf{u} - K\mathbf{v}\|_{M_g} \leq \frac{1}{2}\|\mathbf{u} - \mathbf{v}\|_{M_g}. \quad (3.6)$$

By the Banach contraction mapping principle, there exists a unique solution of the IVP for (3.3)  $\bar{\mathbf{u}} \in M_g \subset C(0, \tau; L^\infty(I))$ . Using  $\bar{\mathbf{u}}(\tau)$  as the initial condition, the local solution can be extended to  $[0, 2\tau]$ , and by repeating this argument to  $[0, T]$  for any  $T > 0$ . In a similar fashion, we can prove the existence and uniqueness of the solution of the IVP for (3.3) on  $[-T, 0]$  for any  $T > 0$ . Furthermore, since the integrand in (3.4) is continuous as a map  $L^\infty(I) \rightarrow L^\infty(I)$ ,  $\mathbf{u}$  is continuously differentiable. Thus, we have a classical solution of the IVP for (3.3) on the whole real axis.

□

### 3.3 Spatial regularity

The classical heat equation is a parabolic partial differential equation. As other equations of this class, it has a strong smoothening property. Regardless of the regularity of the initial data, the solution of the IVP for the classical heat equation is a smooth function of the space variables for all positive times. No such mechanism is present in the heat equation on graph limit. Below we show that the spatial regularity of solutions of the IVP is determined by the regularity of graphon  $W$  and initial condition  $\mathbf{u}(0)$ .

**Theorem 3.2.** *Let  $D : \mathbb{R} \rightarrow \mathbb{R}$  be a Lipschitz continuous function and  $J = (\alpha, \beta) \subset I$ . Suppose  $W \in L^\infty(I^2)$  has a weak derivative  $\frac{\partial}{\partial x} W(x, y)$  for all  $x \in J$  and for almost all  $y \in I$ ; and*

$$\text{ess sup}_{y \in I} \left\| \frac{\partial}{\partial x} W(\cdot, y) \right\|_{L^2(J)} \leq C_1. \quad (3.7)$$

*Then for any  $0 < T < \infty$ , all  $t \in [0, T]$ , and  $\alpha < \alpha' < \beta' < \beta$ , the solution of the IVP for (3.3) satisfies<sup>2</sup>*

$$\mathbf{u}(t) \in H^1(J'), \quad J' = (\alpha', \beta'),$$

*provided  $\mathbf{u}(0) \in L^\infty(I) \cap H^1(J)$ .*

*Proof.* Let

$$h_0 = \frac{1}{2} \min\{\alpha' - \alpha, \beta - \beta'\}.$$

Then for  $0 < h < h_0$ , the difference quotient

$$\xi(x, t) = \frac{u(x + h, t) - u(x, t)}{h}$$

is a well-defined function on  $\Omega_T = J' \times [0, T]$ . Further, for  $(x, t) \in \Omega_T$ ,  $\xi(x, t)$  satisfies the following equation

$$\begin{aligned} \frac{\partial}{\partial t} \xi(x, t) &= \int_I W(x, y) h^{-1} \{D(u(y, t) - u(x + h, t)) - D(u(y, t) - u(x, t))\} dy \\ &+ \int_I D_x^h W(x, y) D(u(y, t) - u(x + h, t)) dy, \end{aligned} \quad (3.8)$$

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<sup>2</sup>  $H^1(J)$  stands for the Sobolev space of all Lebesgue measurable functions  $f$  on an open interval  $J \subset \mathbb{R}^1$  such that  $f$  and its distributional derivative  $f_x$  are in  $L^2(J)$  [6].



where

$$D_x^h W(x, y) = \frac{W(x + h, y) - W(x, y)}{h}.$$

By multiplying both sides of (3.8) by  $\xi(x, t)$  and integrating both sides of the resultant equation over  $J'$  with respect to  $x$ , we have

$$\begin{aligned} \frac{1}{2} \int_{J'} \frac{\partial}{\partial t} \xi(x, t)^2 dx &= \int_{J' \times I} W(x, y) h^{-1} \{D(u(y, t) - u(x + h, t)) - D(u(y, t) - u(x, t))\} \xi(x, t) dx dy \\ &+ \int_{J' \times I} D_x^h W(x, y) D(u(y, t) - u(x + h, t)) \xi(x, t) dx dy \\ &=: T_1 + T_2. \end{aligned} \quad (3.9)$$

Without loss of generality, we assume

$$\|W\|_{L^\infty(I^2)} \leq 1. \quad (3.10)$$

Using  $\mathbf{u} \in C(0, T; L^\infty(I))$ , Lipschitz continuity of  $D(\cdot)$ , and the triangle inequality, we have

$$\max_{t \in [0, T]} \text{ess sup}_{(x, y) \in I^2} |D(u(y, t) - u(x, t))| \leq 2L \|\mathbf{u}\|_{C(0, T; L^\infty(I))} =: C_2. \quad (3.11)$$

Furthermore, using Fubini's theorem, (3.7), and the standard results for the difference quotients (see, e.g., Theorem 5.8.3 [10]), we have

$$\|D_x^h W\|_{L^2(J' \times I)} \leq \text{ess sup}_{y \in I} \|D_x^h W\|_{L^2(J')} \leq C_3 \text{ess sup}_{y \in I} \|W(\cdot, y)\|_{L^2(J)} \leq C_4, \quad (3.12)$$

and, likewise,

$$\|\xi(0)\|_{L^2(J')} \leq C_5 \|\mathbf{u}(0)\|_{H^1(J)}, \quad (3.13)$$

for all  $0 < h < h_0$  and constants  $C_4$  and  $C_5$  independent of  $h \in (0, h_0)$ .

Using (3.10) and (3.2), we bound the first term on the right hand side (3.9)

$$|T_1| \leq \int_{J' \times I} L \xi(x, t)^2 dx dy = L \|\xi(t)\|_{L^2(J')}^2. \quad (3.14)$$

For the second term, we use (3.11), (3.12), and the Cauchy-Schwarz inequality

$$\begin{aligned} |T_2| &\leq C_2 \int_{J' \times I} |D_x^h W \xi(t)| dx dy \leq C_2 \|D_x^h W\|_{L^2(J' \times I)} \|\xi(t)\|_{L^2(J')} \\ &\leq C_2 C_4 \|\xi(t)\|_{L^2(J')}. \end{aligned} \quad (3.15)$$

By combining (3.9), (3.14), and (3.15), we have

$$\frac{d}{dt} \|\xi(t)\|_{L^2(J')}^2 \leq (2L + C_6) \|\xi(t)\|_{L^2(J')}^2 + C_6, \quad C_6 = C_2 C_4,$$

where inequality  $2\|\xi(t)\|_{L^2(J')} \leq \|\xi(t)\|_{L^2(J')}^2 + 1$  was used. Using the Gronwall's inequality, we obtain

$$\begin{aligned} \|\xi(t)\|_{L^2(J')}^2 &\leq \left( \|\xi(0)\|_{L^2(J')}^2 + \frac{C_6}{2L + C_6} \right) \exp\{(2L + C_6)T\} \\ &\leq \left( C_5^2 \|\mathbf{u}(0)\|_{H^1(J)}^2 + \frac{C_6}{2L + C_6} \right) \exp\{(2L + C_6)T\}, \quad t \in [0, T]. \end{aligned} \quad (3.16)$$

The last inequality yields a uniform in  $h \in (0, h_0]$  bound on the difference quotient  $\|\xi(t)\|_{L^2(J')}$ . Using the properties of the difference quotients (cf. Theorem 5.8.3 [10]), we conclude that  $\mathbf{u}(t) \in H^1(J')$  for all  $t \in (0, T]$ .

□

## 4 Networks on simple graphs

As we have seen in the example of the coupled system (1.1) and its continuum limit (1.2), graph limits can be used to guess a candidate for the continuum limit of dynamical networks on convergent sequences of dense graphs. Recall that the kernel  $[W_G]$  in (1.2), the continuum limit of (1.1), was, in fact, the graph limit of the sequence of graphs that was used in (1.1). This leads to a question whether this is true in general. In this section, we initiate the study of this hypothesis for the nonlinear heat equation for certain families of simple graphs. Networks on weighted graphs are considered in the next section.<sup>3</sup>

In this and in the following sections, we prove that the solution of the IVP for appropriately chosen continuous problem (3.3) approximates the solutions of the discrete problems (3.1) when  $n$  is sufficiently large. We prove this result for two classes of convergent graph sequences. In this section, we consider the case of a sequence of simple graphs converging to a  $\{0, 1\}$ -valued graphon, and we study a more general case of convergent sequences of weighted graphs in the next section. We single out networks on  $\{0, 1\}$ -valued graphons for two reasons. First, many coupled oscillator models fit into this framework (see, e.g., [37, 13] and §6.2). Second, for this class of networks we can explicitly estimate the accuracy of approximation of the solutions of the discrete models by those of their continuum limits in terms of the network size and the geometry of the graphon of the network (cf. Theorem 4.1). This result is important, because it reveals the structural properties of the graphs shaping the accuracy of the thermodynamic limit.

After these preliminary remarks, we turn to describe the class of networks to be studied in the remainder of this section. Let  $W : I^2 \rightarrow \{0, 1\}$  be a symmetric measurable function. We denote the support of  $W$  by

$$W^+ = \{(x, y) \in I^2 : W(x, y) \neq 0\}$$

and its boundary by  $\partial W^+$ .

For convenience, we rewrite the IVP for (3.3)

$$\frac{\partial}{\partial t} u(t, x) = \int_I W(x, y) D(u(y, t) - u(x, t)) dy, \quad (4.1)$$

$$u(x, 0) = g(x). \quad (4.2)$$

Throughout this section, to simplify presentation we assume that  $g(x)$  is an interval step function.

Next, we define a sequence of discrete problems. To this end, we fix  $n \in \mathbb{N}$ , divide  $I$  into  $n$  subintervals

$$I_1^{(n)} = \left[0, \frac{1}{n}\right), I_2^{(n)} = \left[\frac{1}{n}, \frac{2}{n}\right), \dots, I_n^{(n)} = \left[\frac{n-1}{n}, 1\right), \quad (4.3)$$

---

<sup>3</sup>For weighted graphs, one can also define convergence by extending the notion of the homomorphism density for this case (see [19] for details). We do not discuss this generalization here, because for the problems that we study in this paper a simpler (and stronger) form of convergence, convergence in  $L^1$ -norm, is sufficient (see Section 5).

and define a sequence of simple graphs  $G_n = \langle V(G_n), E(G_n) \rangle$  such that  $V(G_n) = [n]$  and

$$E(G_n) = \{(i, j) \in [n]^2 : (I_i^{(n)} \times I_j^{(n)}) \cap W^+ \neq \emptyset\}.$$

The IVP for the nonlinear heat equation on  $\{G_n\}$ , a discrete counterpart of (4.1), is given by

$$\frac{d}{dt} u_i^{(n)}(t) = n^{-1} \sum_{j: ij \in E(G_n)} D(u_j^{(n)} - u_i^{(n)}), \quad (4.4)$$

$$u_i^{(n)}(0) = g_i^{(n)}, \quad i \in [n]. \quad (4.5)$$

To compare the solutions of the discrete and continuous models, it is convenient to represent the discrete function  $u^{(n)} = (u_1^{(n)}, u_2^{(n)}, \dots, u_n^{(n)})^\top$  as a step function on  $I$  as follows

$$u_n(x, t) = u_i^{(n)}, \quad \text{if } x \in I_i^{(n)}. \quad (4.6)$$

Then  $u_n(x, t)$  satisfies the following IVP

$$\frac{\partial}{\partial t} u_n(t, x) = \int_I \hat{W}_n(x, y) D(u_n(y, t) - u_n(x, t)) dy, \quad (4.7)$$

$$u(x, 0) = g_n(x), \quad (4.8)$$

where

$$\hat{W}_n(x, y) = \begin{cases} 1, & (I_i^{(n)} \times I_j^{(n)}) \cap W^+ \neq \emptyset, \\ 0, & \text{otherwise} \end{cases} \quad \text{if } (x, y) \in I_i^{(n)} \times I_j^{(n)}, \quad (i, j) \in [n]^2,$$

and

$$g_n(x) = g_i^{(n)} \quad \text{if } x \in I_i^{(n)}, \quad i \in [n].$$

There are many ways for approximating  $g(x)$  by  $g_n(x)$ . For concreteness, we assign  $g_i^{(n)}$  the average value of  $g(x)$  on  $I_i$ :

$$g_i^{(n)} = n^{-1} \int_{I_i^{(n)}} g(x) dx. \quad (4.9)$$

**Theorem 4.1.** *Let  $\mathbf{u}$  and  $\mathbf{u}_n$  denote the vector-valued functions corresponding to the solutions of (4.1), (4.2), and (4.7)-(4.9) respectively. Then for any  $\epsilon > 0$  and all sufficiently large  $n$*

$$\|\mathbf{u} - \mathbf{u}_n\|_{C(0, T; L^2(I))} \leq C_1 n^{\frac{-(1-b-\epsilon)}{2}}, \quad (4.10)$$

where constant  $C_1$  is independent of  $n$ , and  $2b = \overline{\dim}_B \partial W^+$  is the upper box-counting dimension of  $\partial W^+$  (cf. § 3.1, [11]).

*Proof.* Denote  $\xi_n(x, t) = u_n(x, t) - u(x, t)$ . By subtracting (4.1) from (4.7), we have

$$\begin{aligned} \frac{\partial \xi_n}{\partial t} &= \int_I \hat{W}_n(x, y) \{D(u_n(y, t) - u_n(x, t)) - D(u(y, t) - u(x, t))\} dy \\ &+ \int_I (\hat{W}_n(x, y) - W(x, y)) D(u(y, t) - u(x, t)) dy. \end{aligned} \quad (4.11)$$

Next, we multiply both sides of (4.11) by  $\xi_n(x, t)$  and integrate over  $I$

$$\begin{aligned} \frac{1}{2} \int_I \frac{\partial}{\partial t} \xi_n(x, t)^2 dx &= \int_{I \times I} \hat{W}_n(x, y) \{D(u_n(y, t) - u_n(x, t)) - D(u(y, t) - u(x, t))\} \xi_n(x, t) dx dy \\ &+ \int_{I \times I} (\hat{W}_n(x, y) - W(x, y)) D(u(y, t) - u(x, t)) \xi_n(x, t) dx dy. \end{aligned} \quad (4.12)$$

Using the Lipschitz continuity of  $D(\cdot)$ ,  $\|\hat{W}\|_{L^\infty(I^2)} = 1$ , the triangle inequality, and the Cauchy-Schwarz inequality, we estimate the first term on the right-hand side of (4.12)

$$\begin{aligned} &\left| \int_{I \times I} \hat{W}_n(x, y) \{D(u_n(y, t) - u_n(x, t)) - D(u(y, t) - u(x, t))\} \xi_n(x, t) dx dy \right| \\ &\leq L \int_{I \times I} |(\xi_n(y, t) - \xi_n(x, t)) \xi_n(x, t)| dx dy \leq 2L \|\xi_n(t)\|_{L^2(I^2)}^2. \end{aligned} \quad (4.13)$$

We estimate the second term on the right-hand side of (4.12), using the Cauchy-Schwarz inequality and the bound on  $D(\cdot)$  (cf. (3.11))

$$\begin{aligned} &\left| \int_{I^2} (\hat{W}_n(x, y) - W(x, y)) D(u(y, t) - u(x, t)) \xi_n(x, t) dx dy \right| \\ &\leq \text{ess sup}_{(x, y, t) \in I^2 \times [0, T]} |D(u(y, t) - u(x, t))| \left| \int_{I^2} (\hat{W}_n(x, y) - W(x, y)) \xi_n(x, t) dx dy \right| \\ &\leq C_2 \|W - \hat{W}_n\|_{L^2(I^2)} \|\xi_n\|_{L^2(I)} \end{aligned} \quad (4.14)$$

for some constant  $C_2 > 0$  independent of  $n$ .

Using (4.13) and (4.14), from (4.12) we have

$$\begin{aligned} \frac{d}{dt} \|\xi_n\|_{L^2(I)}^2 &\leq 4L \|\xi_n\|_{L^2(I)}^2 + 2C_2 \|W - \hat{W}_n\|_{L^2(I^2)} \|\xi_n\|_{L^2(I)} \\ &\leq (4L + C_2 \|W - \hat{W}_n\|_{L^2(I^2)}) \|\xi_n\|_{L^2(I)}^2 + C_2 \|W - \hat{W}_n\|_{L^2(I^2)}. \end{aligned} \quad (4.15)$$

To estimate  $\|W - \hat{W}_n\|_{L^2(I^2)}$ , consider the set of discrete cells  $I_i^{(n)} \times I_j^{(n)}$  that covers the boundary of the support of  $W$

$$J(n) = \{(i, j) \in [n]^2 : (I_i^{(n)} \times I_j^{(n)}) \cap \partial W^+ \neq \emptyset\} \text{ and } C(n) = |J(n)|.$$

Using one of several equivalent definitions of the upper box-counting dimension of a subset of  $\mathbb{R}^n$ , we have

$$2b := \overline{\dim}_B \partial W^+ = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(\partial W^+)}{-\log \delta},$$

where  $N_\delta(\partial W^+)$  is the number of cells of a  $(\delta \times \delta)$ -mesh that intersect  $\partial W^+$  (see Equation (3.12)(iv) in [11]). Thus, for any  $\epsilon > 0$  and all sufficiently large  $n$ , we have

$$C(n) \leq n^{2(b+\epsilon)}.$$

Since  $W$  and  $\hat{W}_n$  coincide on all cells  $I_i^{(n)} \times I_j^{(n)}$  for which  $(i, j) \notin J(n)$ , for any  $\epsilon > 0$  and all sufficiently large  $n$ , we have

$$\|W - \hat{W}_n\|_{L^2(I^2)}^2 = \int_{I^2} (W - \hat{W}_n)^2 dx dy \leq C(n)n^{-2} \leq n^{-2(1-b-\epsilon)}. \quad (4.16)$$

In particular,

$$\|W - \hat{W}_n\|_{L^2(I^2)} \leq C_3, \quad (4.17)$$

for some positive constant  $C_3$  independent of  $n$ .

By plugging (4.17) into (4.15), we have

$$\frac{d}{dt} \|\xi_n\|_{L^2(I)}^2 \leq C_4 \|\xi_n\|_{L^2(I)}^2 + C_2 \|W - \hat{W}_n\|_{L^2(I^2)}, \quad C_4 = 4L + C_2 C_3, \quad (4.18)$$

where positive constants  $C_2$  and  $C_4$  do not depend on  $n$ . By Gronwall's inequality, from (4.18) we have

$$\sup_{t \in [0, T]} \|\xi_n(t)\|_{L^2(I)}^2 \leq \left( \|\mathbf{g} - \mathbf{g}_n\|_{L^2(I)}^2 + \frac{C_2 \|W - \hat{W}_n\|_{L^2(I^2)}}{C_4} \right) \exp\{C_4 T\}. \quad (4.19)$$

Finally, from (4.9) it is easy to see that

$$\|\mathbf{g} - \mathbf{g}_n\|_{L^2(I)}^2 = O(n^{-1}) \quad (4.20)$$

The combination of (4.19), (4.16), and (4.20) implies (4.10).

□

## 5 Networks on weighted graphs

In this section, we study a more general case of the heat equation on convergent sequences of weighted graphs. First, we define two graph sequences generated by a given graphon  $W$  and then we prove the convergence of the corresponding discrete problems to the continuum limit (4.1).

Throughout this section, we assume that  $W : I^2 \rightarrow [-1, 1]$  is a symmetric measurable function. Let  $\mathcal{P}_n$  denote the partition of  $I$  into  $n$  intervals,  $\mathcal{P}_n = \{I_i^{(n)}, i \in [n]\}$  (see (4.3)) and

$$X_n = \left\{ \frac{1}{n}, \frac{2}{n}, \dots, \frac{n}{n} \right\}.$$

The quotient of  $W$  and  $\mathcal{P}_n$ , denoted  $W/\mathcal{P}_n$ , is the complete graph on  $n$  nodes

$$W/\mathcal{P}_n = \langle [n], [n] \times [n], \bar{W}_n \rangle,$$

such that weights  $(\bar{W}_n)_{ij}$  are obtained by averaging  $W$  over the sets in  $\mathcal{P}_n$

$$(\bar{W}_n)_{ij} = n^2 \int_{I_i \times I_j} W(x, y) dx dy. \quad (5.1)$$

The second sequence of weighted graphs is obtained in a way that is similar to the construction of  $W$ -random graph (cf. Example 2.4)

$$\mathbb{H}(S_n, W) = \langle [n], [n] \times [n], \tilde{W}_n \rangle, (\tilde{W}_n)_{ij} = W\left(\frac{i}{n}, \frac{j}{n}\right). \quad (5.2)$$

In the remainder of this section, we prove convergence of the nonlinear heat equations on  $W/\mathcal{P}_n$  and  $\mathbb{H}(S_n, W)$  to the continuum equation on the graphon  $W$  (cf. (4.1)). Furthermore, we show that the former problems correspond to the discretizations of (4.1) using the method of Galerkin and the collocation method respectively, thus, relating the problem of justification of the thermodynamic limit for dynamical networks to two well-known numerical schemes for equations of mathematical physics.

We first consider the IVP for the heat equation on  $W/\mathcal{P}_n$

$$\frac{d}{dt}u_i^{(n)}(t) = n^{-1} \sum_{j=1}^n (\tilde{W}_n)_{ij} D\left(u_j^{(n)}(t) - u_i^{(n)}(t)\right), \quad (5.3)$$

$$u_i^{(n)}(0) = g_i^{(n)}, \quad i \in [n] \quad (5.4)$$

where  $g_i^{(n)}$  is defined in (4.9).

By associating the step function  $u_n(x, t)$  with  $u^{(n)}(t)$  (see (4.6)), we rewrite (5.3) and (5.4) as

$$\frac{\partial}{\partial t}u_n(x, t) = \int_I W_n(x, y) D(u_n(y, t) - u_n(x, t)) dy, \quad (5.5)$$

$$u_n(x, 0) = g_n(x), \quad (5.6)$$

where  $W_n$  and  $g_n$  are the step functions

$$\begin{aligned} W_n(x, y) &= \bar{W}_{ij} \text{ for } (x, y) \in I_i^{(n)} \times I_j^{(n)}, \\ g_n(x) &= g_i^{(n)}, \text{ for } x \in I_i^{(n)}. \end{aligned}$$

While we do not use this fact explicitly, it is instructive to note that (5.3) and (5.4) can be viewed as the Galerkin approximation of the IVP (4.1) and (4.2). Indeed, let  $H_n$  denote a finite-dimensional subspace of  $L^2(I)$

$$H_n = \text{span}\{\phi_1, \phi_2, \dots, \phi_n\},$$

where  $\phi_i = \chi_{I_i^{(n)}}$  is the characteristic function of  $I_i^{(n)} = [(i-1)n^{-1}, in^{-1})$ .

Replacing  $u(x, t)$  in (4.1) with

$$u_n(x, t) = \sum_{k=1}^n u_k^{(n)}(t) \phi_k(x) \in H_n$$

and projecting the resultant equation on  $H_n$ , we arrive at (5.3).

**Theorem 5.1.** *Let  $\mathbf{u}$  and  $\mathbf{u}_n$  be the solutions of (4.1), (4.2), and (5.5), (5.6), respectively. Suppose  $W \in L^\infty(I^2)$  and  $\mathbf{g} \in L^\infty(I)$ . Then*

$$\|\mathbf{u} - \mathbf{u}_n\|_{C(0,T;L^2(I))} \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (5.7)$$

*Proof.* By following the lines of the proof of Theorem 4.1 (see (4.19)), for  $\xi_n(x, t) = u_n(x, t) - u(x, t)$  we obtain

$$\sup_{t \in [0, T]} \|\xi_n(t)\|_{L^2(I)} \leq \left( \|\mathbf{g} - \mathbf{g}_n\|_{L^2(I)}^2 + \frac{C_1 \|W - W_n\|_{L^2(I^2)}}{C_2} \right) \exp\{C_2 T\}, \quad (5.8)$$

where positive constants  $C_1$  and  $C_2$  are independent of  $n$ . By the Lebesgue differentiation theorem,

$$W_n \rightarrow W \text{ and } \mathbf{g}_n \rightarrow \mathbf{g}, \text{ as } n \rightarrow \infty,$$

almost everywhere on  $I^2$  and  $I$  respectively. Thus, the statement of the theorem follows from (5.8).  $\square$

The heat equation on  $\mathbb{H}(X_n, W)$  is analyzed in complete analogy to the IVP for  $W/\mathcal{P}_n$ . The IVP in this case remains (5.5) and (5.6) modulo the definition of the step function

$$W_n(x, y) = \tilde{W}_{ij} \text{ for } (x, y) \in I_i^{(n)} \times I_j^{(n)}. \quad (5.9)$$

We assume that  $W(x, y)$  is a bounded symmetric measurable function that is almost everywhere continuous on  $I^2$ . Then using the observation in Lemma 2.5 [3],

$$W_n(x, y) \rightarrow W(x, y), \text{ as } n \rightarrow \infty$$

at every point of continuity of  $W$ , i.e., almost everywhere. Thus, by the dominated convergence theorem, we have

$$\|W - W_n\|_{L^2(I^2)} \rightarrow 0 \text{ as } n \rightarrow \infty.$$

With this observation, the proof of Theorem 5.1 applies to the situation at hand. Thus, we have the following theorem.

**Theorem 5.2.** *Let  $\mathbf{u}$  and  $\mathbf{u}_n$  be the solutions of (4.1), (4.2), and (5.5), (5.9), (5.6), respectively. Suppose  $W \in L^\infty(I^2)$ ,  $\mathbf{g} \in L^\infty(I)$ , and  $W$  is continuous almost everywhere on  $I^2$ . Then*

$$\|\mathbf{u} - \mathbf{u}_n\|_{C(0,T;L^2(I))} \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (5.10)$$

## 6 Examples

In this section, we illustrate the results of this paper with three examples. First, we apply Theorem 3.2 to explain the regions of continuity in chimera states. Next, we discuss the attractors of the system of Kuramoto oscillators on the bipartite complete graph and on the half-graph.

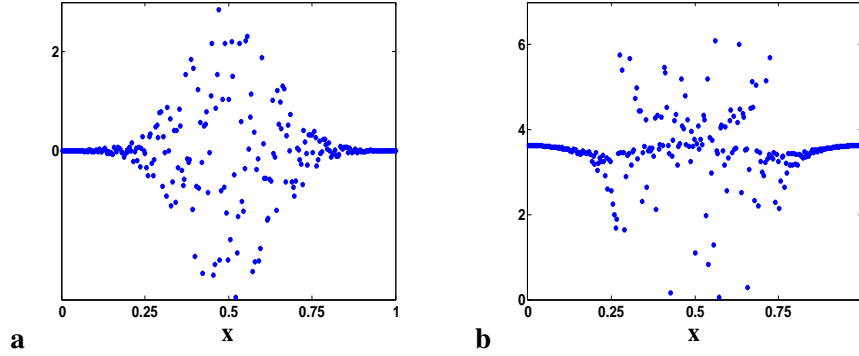


Figure 2: a) The initial conditions (6.2) for the chimera state shown in b). b) A snapshot of the chimera state generated by (6.1).

## 6.1 Regions of continuity of chimera states

Chimera states are persistent patterns of coexisting regions of spatially coherent and chaotic behaviors (see Fig. 2a). They were found by Kuramoto and Battogtokh in the following continuum limit of a system of coupled phase oscillators [15]

$$\frac{\partial}{\partial t} \phi(x, t) = \omega + \int_0^1 G(x - y) \sin(\phi(y, t) - \phi(x, t) + \alpha) dy. \quad (6.1)$$

Function  $\phi : [0, 1] \times \mathbb{R}^+ \rightarrow \mathbb{S}^1 := \mathbb{R}/2\pi\mathbb{Z}$  describes the evolution of the phase of oscillator at  $x \in [0, 1]$ . The exponential kernel  $G(x) = \exp\{-\kappa|x|\}$  provides nonlocal coupling between oscillators. Equation (6.1) was obtained using the phase reduction from the Ginzburg-Landau equation, which describes collective dynamics of nonlocally coupled limit cycle oscillators (cf. [15]). The sequences of discrete problems converging to (6.1) can be obtained using one of the schemes of Section 5.

The numerical generation of the chimera state requires a careful setup, which we review next. To trigger a chimera state one has to start with the appropriate initial conditions, otherwise oscillators end up evolving in phase. Abrams and Strogatz reported that they were unable to generate chimera states from smooth initial conditions [1]. Instead, one has to initialize the system with the initial condition that combines the regions of coherent and incoherent spatial profiles. The following initial condition was suggested by Kuramoto (cf. [1]):

$$\phi(x_i, 0) = h(x_i)r_i, \text{ where } h(x) = 6 \exp\left\{-30(x - (1/2))^2\right\}, \quad x_i = in^{-1}, \quad i \in [n], \quad (6.2)$$

and  $r_i$  are independent random variables drawn from the uniform distribution on  $(-1/2, 1/2)$  (see Fig. 2a). The values of the other parameters are  $\kappa = 4$ ,  $\alpha = 1.457$  (cf. [1]). Numerical integration of (6.1) and (6.2) with these parameter values yields persistent patterns with coexisting regions of spatially coherent and chaotic dynamics. A representative snapshot is shown in Fig. 2b.

Theorem 3.2 explains the role of the initial conditions in generating chimera states. Note that function  $h(x)$  in (6.2) is rapidly decaying to 0 outside a neighborhood of  $1/2$ . Therefore, the initial conditions in the intervals  $J_1 = (0, 0.2)$  and  $J_2 = (0.8, 1)$  near the endpoints of the interval  $[0, 1]$  for all practical purposes can be viewed if they were produced by discretization of a function that is smooth over  $J_1$  and  $J_2$  (see



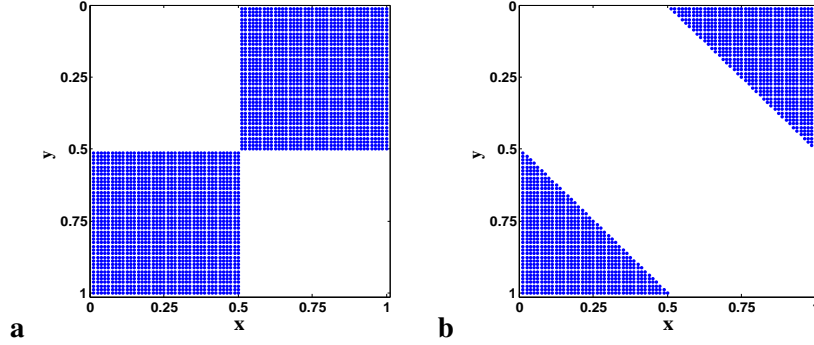


Figure 3: The graphons representing the limits of the families of the complete bipartite graphs  $K_{n,n}$  (a) and the half graphs  $H_{n,n}$  (b).

Fig. 2b). For such initial conditions, Theorem 3.2 implies that the solution  $\phi(x, t)$  will remain continuous on  $J_1$  and  $J_2$ , because  $H^1(J_{1,2}) \subset C(J_{1,2})$  by the Sobolev Embedding Theorem. This explains why the spatial profile remains coherent over  $J_1$  and  $J_2$  for positive times (see Fig. 2a). Theorem 3.2 also implies that it is impossible to generate chimera states starting from smooth initial data, because for such data the solution of the continuum limit remains continuous over the entire domain for all  $t > 0$ . This rules out regions of chaotic behavior in large networks, because their solutions remain close to that of the continuous system by Theorem 5.1 or Theorem 5.2. This explains why one can not produce chimera states from smooth initial conditions in [1].

## 6.2 The Kuramoto equation on bipartite graphs

To illustrate our results for networks on simple graphs, in this subsection we discuss the Kuramoto equation on the two families of bipartite graphs: the complete bipartite graphs  $\{K_{n,n}\}$  and the half-graphs  $\{H_{n,n}\}$ . The half-graph  $H_{n,n}$  was defined in Example 2.5. The complete bipartite graph  $K_{n,n} = \langle [2n], E(K_{n,n}) \rangle$ , where

$$(i, j) \in E(K_{n,n}) \text{ whenever } 1 \leq i \leq n < j \leq 2n.$$

Both graph sequences are convergent with the limits shown in Fig. 3.

Consider the Kuramoto equation on  $K_{n,n}$

$$\dot{u}_i^{(n)}(t) = \frac{\sigma}{n} \sum_{j: (j,i) \in E(K_{n,n})} \sin(u_j^{(n)}(t) - u_i^{(n)}(t)), \quad i \in [2n], \quad (6.3)$$

where  $u_i^{(n)} : \mathbb{R} \rightarrow \mathbb{S}^1$ . We consider two models for  $\sigma = 1$  and  $\sigma = -1$ . As shown below, the space homogeneous (synchronous) solution is stable for the  $\sigma = 1$  model and is unstable if  $\sigma = -1$ .

Along with (6.3) we consider its continuum limit

$$\frac{\partial}{\partial t} u(x, t) = \sigma \int_I K(x, y) \sin(u(y, t) - u(x, t)) dy, \quad (6.4)$$

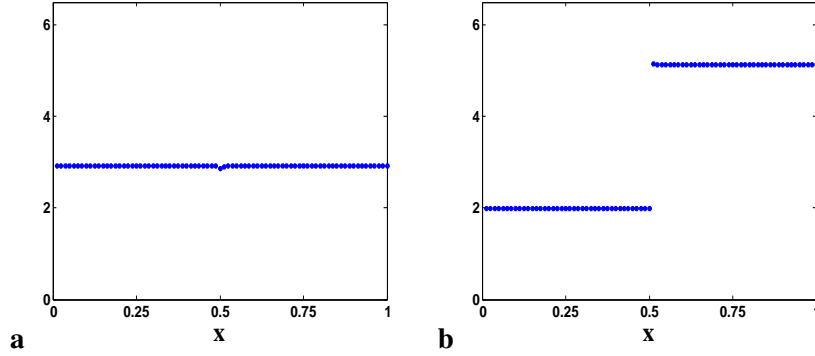


Figure 4: Solutions of the IVP problem for the Kuramoto equation on the half- and bipartite complete graphs converge to the synchronous solution for  $\sigma = 1$  (a) and to the step function for  $\sigma = -1$  (b).

where graphon  $K \in \mathcal{W}_0$  is the limit of  $\{K_{n,n}\}$  (see Fig. 3a). Suppose  $u(x, 0) \in C(I)$ . By Theorem 3.2, for any  $t > 0$ ,  $u(x, t) \in \tilde{C}(I)$  where

$$\tilde{C}(I) = \{u \in L^\infty(I) : \text{for any open interval } J \subset (0, 1/2) \cup (1/2, 1) \text{ } u|_J \in C(J)\}.$$

Here, by  $u|_J$  we denote the restriction of  $u$  to  $J$ .

We look for steady state solutions of (6.4) that belong to  $\tilde{C}(I)$ . Setting the right hand side of (6.4) to 0, we obtain

$$\int_{1/2}^1 \sin(u(y, t) - u(x, t)) dy = 0, \quad x \in (0, 1/2), \quad (6.5)$$

$$\int_0^{1/2} \sin(u(y, t) - u(x, t)) dy = 0, \quad x \in (1/2, 1). \quad (6.6)$$

From (6.5) and (6.6), we find that the only steady state solutions from  $\tilde{C}(I)$  are the space homogeneous function

$$u^h(x) = c, \text{ for } x \in [0, 1],$$

and the step function

$$u^s(x) = \begin{cases} c_1, & x \in [0, 1/2), \\ c_2, & x \in [1/2, 1], \end{cases}$$

where constants  $c, c_1, c_2 \in \mathbb{S}^1$  and  $|c_2 - c_1| = \pi/2$ .

Next, we turn to the discrete model (6.3). The discrete counterparts of  $u^s(x, t)$  and  $u^h(x, t)$  are

$$u^s = c \mathbf{1}_{2n} \in \mathbb{R}^{2n} \text{ and } u^h = (c_1 \mathbf{1}_n^\top, c_2 \mathbf{1}_n^\top) \in \mathbb{R}^{2n},$$

where  $\mathbf{1}_n = (1, 1, \dots, 1)^\top \in \mathbb{R}^n$ .

The linearization of (6.3) about  $u = u^h$  yields

$$\dot{\xi} = -\frac{\sigma}{n} \mathbf{L} \xi. \quad (6.7)$$

Matrix  $\mathbf{L}$  is the Laplacian of the half graph  $H_{n,n}$

$$\mathbf{L} = \begin{pmatrix} nI_n & -J_n \\ -J_n & nI_n \end{pmatrix}, \quad (6.8)$$

where  $I_n$  is the  $n \times n$  identity matrix and  $J_n = \mathbf{1}_n \mathbf{1}_n^\top$ . As a graph Laplacian of an undirected connected graph,  $\mathbf{L}$  is a symmetric positive semi-definite matrix with a simple 0 eigenvalue [12]. Thus, the space homogeneous solution  $u^h$  is neutrally linearly stable for  $\sigma = 1$  and is unstable when  $\sigma = -1$ .

The linearization of (6.3) about  $u^s$  yields

$$\dot{\xi} = \frac{\sigma}{n} \mathbf{L} \xi,$$

which up to a sign coincides with (6.7). Thus,  $u^s$  is unstable if  $\sigma = 1$  and is neutrally stable for  $\sigma = -1$ .

Note that both families of synchronous and the step function steady state solutions,  $u^h$  and  $u^s$ , are invariant under the perturbations along the center direction  $\text{span}\{\mathbf{1}_{2n}\}$ . This suggests that both solutions persist under these perturbations, i.e., the synchronous and step steady states are stable for  $\sigma = 1$  and  $\sigma = -1$  respectively.<sup>4</sup> Note that the discrete model (6.3) has many other steady state solutions besides  $u^h$  and  $u^s$ . But the latter are the only two that approximate functions in  $\tilde{C}(I)$  and, therefore, only these solutions can be attractors of the discrete system for large  $n$  (cf. Theorem 3.2). This conclusion is consistent with the numerical simulations shown in Fig. 4. Numerical experiments show that the synchronous state is the attractor for the Kuramoto model with  $\sigma = 1$ , while the step function is the attractor for the model with  $\sigma = -1$  (see Fig. 4b,c).

The analysis of the Kuramoto equation on the family of half-graphs follows the same lines with obvious modifications. It is interesting to note, however, that Theorem 3.2 does not apply to the heat equation on the half-graphs. Nonetheless, the Kuramoto equation on the family of the half-graph exhibit the same attractors as in the case of the complete bipartite graphs.

## 7 Conclusion

The heat equation is one of the most fundamental equations of mathematical physics. On Euclidean domains, the heat operator is used to model many important phenomena involving diffusion, propagation, and pattern formation in diverse problems of physics and biology. On Riemannian manifolds, the heat equation has been a powerful tool for studying the topology of the underlying manifold [32]. Its discrete counterpart, the heat equation on graphs plays an important role in the spectral graph theory [7].

Motivated by the problems of the dynamics of large networks, in this paper we have introduced and studied the nonlinear heat equation on graphs. For convergent sequences of dense graphs, we derived the heat equation on graph limits and showed that it approximates the dynamics of sufficiently large networks. The heat equation on the graph limit is an integro-differential equation with the kernel of the integral operator given by the graphon, a symmetric bounded measurable function, which represents the limit of the underlying graph sequence.

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<sup>4</sup>The rigorous stability analysis requires a center manifold reduction. This is beyond the scope of this paper (see [25, 23] for the analysis of closely related models).

We studied two classes of networks on convergent graph sequences: the family of networks on simple graphs that converge to a  $\{0, 1\}$ -valued graphon and two families of networks on weighted graphs. In each case, we have proved convergence of solutions of the discrete problems on graphs to those of the continuous problems on graph limits. For the case of simple graphs, we have also estimated the rate of convergence in terms of the network size and the upper box counting dimension of the boundary of support of the graph limit. This result provides the link between the geometry of graphons and the accuracy of the thermodynamic limit approximation of large networks. For networks on weighted graphs considered in this paper, we also show that they can be interpreted as the discretizations of the continuum limit via the method of Galerkin or the collocation method.

The results of this paper are illustrated with two examples. First, we explain the regions of continuity in the chimera states, the counterintuitive solutions of the systems of coupled phase oscillators. Next, we study the attractors in the Kuramoto coupled oscillators equation model on the complete bipartite graph and on the half graph. Both examples highlight the qualitative differences between solutions of the classical heat equation and that on the graph limit. While the former are smooth functions of the space variables for all positive times, due to the smoothening property of the parabolic partial differential operators, the latter may be discontinuous, as the examples of the heat equation on the complete bipartite graph shows.

The theory of graph limits provides a useful set of tools for studying dynamics of large networks. On one hand, known graph limits for various convergent sequences like the half graph or  $W$ -random graphs suggest continuum limits for a broad class of large networks. On the other hand, this rich theory offers many useful ideas and analytical results that can be applied to dynamical networks. In this paper, we analyzed three families of networks on convergent sequences of deterministic graphs. In the future work, we will consider networks on convergent sequences of random graphs such as the Erdős-Renyi and the small world graphs, which are ubiquitous in applications [1, 24, 36].

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